

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.50e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.73e-01

Confidence level: 7.51e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,4,6-Trichlorophenol</div> <div>Measured: 8.39e-02</div> <div>Predicted: 1.49e-02</div>	<div>Image not found</div> <div>Butyl methacrylate</div> <div>Measured: 7.00e-02</div> <div>Predicted: 2.42</div>	<div>Image not found</div> <div>4-tert-Butylphenol</div> <div>Measured: 4.23e-02</div> <div>Predicted: 5.13e-02</div>
<div>Image not found</div> <div>Propane, 2-bromo-2-methyl-</div> <div>Measured: 5.02e-02</div> <div>Predicted: 81.9</div>	<div>Image not found</div> <div>4-Chlorophenyl isocyanate</div> <div>Measured: 2.87</div> <div>Predicted: 1.18e-01</div>	